

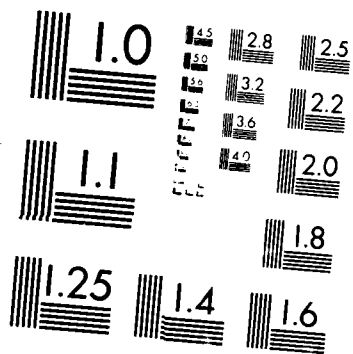
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18 SUBJECT TERMS (Continue on reverse if necessary and identify by block number)

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19 ABSTRACT (Continue on reverse if necessary and identify by block number)

DNA polymer in dilute aqueous solution responds to external illumination. Because it is a charged system surrounded by another charged system, counterions, it interacts strongly electromagnetically. We find that a normal mode may exist in the form of a one dimensional plasmon, analogous to the three dimensional plasmons well known in metal physics and the two dimensional surface plasmons of surface physics of conductors. The DNA plasmon frequency is proportional to the excitation wave number, i.e. the first power, in contrast with the one-half power for surface plasmons and the zero power for bulk metallic plasmons.

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Progress Report

STORING BITS ON A DNA POLYMER CHAIN

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L.L. Van Zandt, P.I.

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Completed Projects:

[1] A detailed exposition of the dynamics of DNA polymer chain dissolved in saline aqueous medium was reported in *Physical Review*. The calculation included the full effects of radially inhomogeneous counter ion distribution, DNA dynamics, Maxwell's equations, counterion currents and charges. Care was taken to allow for different dynamics and interactions with the first hydration layer, a monomolecular surrounding sheath of water having distinct properties from the farther, "bulk" water. A comprehensive range of parameter values for the hydration layer parameters was explored and presented. In some but not all regions of this parameter space, well defined longitudinal compressional waves are to be expected. Hence when the experimental question of the existence of these modes is settled one way or the other, limits will be placed on the DNA-water interaction strengths.

[2] The detailed model of DNA + water + hydration layer + counterion dynamics of the above was explored for the dependence on the ionic strength of the saline solvent and a modest range of temperatures between freezing and DNA denaturing. A curious interference between two effects was found rendering the predicted dynamics almost independent of the temperature over the range considered. Similarly, because the near environment of the DNA is only weakly dependent on the salt concentration of the greater solution, a phenomenon known as the "Manning condensation", the predicted dynamics of the complex system are also very nearly independent of the solvent ionic strength.

[3] The Helmholtz free energy of B-DNA polymer was examined as a function of several parameters describing the structural conformation. Particular attention was paid to the relative orientations of the bases in the individual base pairs, the "propellor twist" angle, and also the orientation of the two base pairs as a unit with respect to the long axis of the double helix. Assuming that the observed X-ray diffraction values of these parameters are the result of a minimum in the free energy, we determined from the vibrational spectrum what the curvature of the potential energy "well" at the bottom had to be. We divided the free energy into two parts, the first one a static potential energy arising from vanDerwaals and Coulomb interactions normally treated by authors seeking to understand and/or predict the equilibrium structure. The second was a new contribution arising from the modification of the thermal occupation of the many vibrational modes as the structure is distorted. We determined that the vibrational terms were a significant contribution to the free energy in comparison with the static potentials, and that the true minima of the static potentials must occur at different coordinate values than the use of static potential functions alone would suggest. Hence, authors seeking to analyze the interatomic potential functions on the basis of structural information make considerable errors if the vibrational mode contributions to the energy minimization process are neglected.

[4] A full cubic centimeter of well oriented DNA polymer has recently been studied by inelastic neutron scattering. A vibrational mode branch of the spectrum was clearly revealed in these studies. We have analyzed the experimental results in terms of compressional wave phonons on the polymer chain. Because the region of frequency/wavelength space sampled by the inelastic neutron technique was well outside the reach of what we normally call the acoustic phonon branch, we projected out the compressional character of the eigenvectors in all the branches up to the 20th and followed the compressional wave as



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it ascended in frequency through the many nominally optical branches of the spectrum. Excellent agreement between the experimental results and the theoretical map was obtained.

[5] The character of the eigenvectors of the complete spectrum of poly dA·poly dT was projected onto a subspace of dynamical motions consisting entirely of homogeneous rotations and translations of large subunits of the dinucleotide monomeric unit, the bases, the sugar rings, and the phosphate groups. We found that up to about 380 cm^{-1} the motion consisted essentially *entirely* of elementary subunit motions whereas above this "cutoff" frequency the motions were essentially *entirely* internal vibrations of the subunits. This clean separation into two frequency regimes implies that little of interest to biological functioning can be expected from excitations above 380 cm^{-1} .

[6] In an effort originally begun to simplify the description of the long range, weak, interatomic forces, we introduced the longitudinal electric field E_z as an explicit dynamical coordinate in the normal mode problem. Maxwell's equations then become part of the system equations of motion. We have found thereby (in addition to the simplification we sought) a new class of excitations, the DNA plasmon. This is basically a longitudinal photon trapped on or guided by the one dimensional charge distribution represented by the DNA polymer chain and its associated sheath of water and counterions.

Work Still in Progress:

[7] We are exploring the dynamics of a long chain polymer with a unit cell consisting of $2\frac{1}{2}$ base pairs, the "five base" model. We expect the results to bear significantly on the central thrust of this contract, the storing of a bit by a missing base defect.

[8] We are continuing to develop calculational techniques to deal with the general problem of the localized defect. The results in [5] above are expected to aid our search substantially.

[9] We are at work on a procedure for describing structural transitions in a novel way. We expect this to bear on the question of manipulating the stored information - the bits - of the base pair defect and also to be relevant to the general problem. We hope to address the B to Z structural transformation.

Papers:

"Microwave Response of DNA in Solution: Theory", M.E. Davis & L.L. Van Zandt, *Phys. Rev.* 37, 888 (1987).

"Temperature and Concentration Behavior of Anomalous Microwave Resonances in DNA", M.E. Davis & L.L. Van Zandt, submitted.

"Helical Lattice Vibrational Modes in DNA", V.V. Prabhu, W.K. Schroll, L.L. Van Zandt, E.W. Prohofsky, *Phys Rev. Lett. Comments* (1988).

"Phonon Interpretation of Inelastic Neutron Scattering in DNA Crystals", W.K. Schroll, V.V. Prabhu, E.W. Prohofsky & L.L. Van Zandt, submitted.

"Biological Significance and Insignificance of DNA Vibrations", L.L. Van Zandt, V.K. Saxena & W.K. Schroll, submitted.

"The DNA Plasmon", L.L. Van Zandt & V.K. Saxena, submitted.

Thesis:

"Theory of the Response by DNA in Solution to Microwave Illumination", Purdue University, M.E. Davis, May, 1987.

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